

Vortex families near a spectral edge in the Gross-Pitaevskii equation with a two-dimensional periodic potential

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We examine numerically vortex families near band edges of the Bloch wave spectrum in the Gross–Pitaevskii equation with a two-dimensional periodic potential and in the discrete nonlinear Schrödinger equation. We show that besides vortex families that terminate at a small distance from the band edges via fold bifurcations there exist vortex families that are continued all way to the band edges.

I. INTRODUCTION

Many physical problems in periodic media with the Kerr (cubic) nonlinearity are governed by the Gross–Pitaevskii equation with a periodic potential. Examples are Bose–Einstein condensates in optical lattices [17] and photonic-crystal fibers [18]. Interest in properties of localized states in this model has stimulated a number of mathematical works devoted to this subject [13, 23].

An interesting problem that arises in this context is the possibility of bifurcations of stationary localized states from edges of Bloch bands in the wave spectrum of the Schrödinger operator with a periodic potential. First pioneering works in this direction were completed by C. Stuart and his students [7, 12, 21]. In the physics literature the asymptotic approximations of gap solitons bifurcating from band edges were developed by various authors in one dimension [8, 16] and two dimensions [9, 19, 20].

In one dimension it was discovered numerically in [23, Chapter 6.2] and explained analytically in [2] that while single-pulse gap solitons bifurcate continuously from band edges, double-pulse gap solitons do not bifurcate from the band edges but experience fold bifurcations at a small distance from the edges. The situation becomes even more interesting in the space of two dimensions, where besides gap solitons, vortex solutions are possible in periodic potentials [5, 6, 22]. However, a contradiction arises between the analytical results of [5, 6] suggesting a continuous family of the fundamental vortex solutions bifurcating from the band edges and the numerical results of [22] (see

also [23, Chapter 6.5]) suggesting a fold bifurcation of vortex families at a small distance from the band edges. This contradiction will be inspected in this paper by using numerical computations.

We will show that there do exist continuous families of the fundamental vortex solutions bifurcating from band edges, according to the theory in [5, 6]. Numerical approximations of these families near band edges suffer, however, from the fact that the vortex localization is too broad and hence extends beyond the chosen computational domain. As a result, a spurious fold bifurcation occurs for the fundamental vortex family before the family reaches the band edge. If the size of the computational domain is enlarged, the location of the spurious fold bifurcation moves closer to the band edge. At the same time there are other vortex families, found also in [22], which feature a true fold bifurcation at a small distance from a band edge. The fold location is independent of the size of the computational domain for these vortex families.

The paper is organized as follows. Section II introduces the two models which we inspect, namely the Gross–Pitaevskii equation with a periodic potential and the discrete nonlinear Schrödinger equation. The connection between these models as well as the asymptotics of gap solitons near the band edges are reviewed. Section III gives numerical results for the family of fundamental vortices. Section IV illustrates fold bifurcations for families of quadrupole and dipole vortex configurations. In Section V we summarize our findings.

II. MODELS

The stationary Gross–Pitaevskii equation with a periodic potential in the space of two dimensions takes the form

$$-\Delta\varphi + V(x, y)\varphi - |\varphi|^2\varphi = \omega\varphi, \quad (x, y) \in \mathbb{R}^2, \quad (\text{II.1})$$

where the focusing case is considered, the 2π -periodic potential V in each coordinate is assumed to be bounded, and $\omega \in \mathbb{R}$ is taken in a spectral gap of the Schrödinger operator

$$L_0 := -\Delta + V.$$

For simplicity, we assume that the periodic potential V has even symmetries with respect to reflections about $x = 0$ and $y = 0$.

When ω is close to the upper edge ω_0 of a spectral gap of L_0 , a slowly varying envelope approximation of localized states can be derived and rigorously justified in the focusing stationary

Gross–Pitaevskii equation [5, 6]. In the simplest case when ω_0 is attained by only one extremum of the band structure and the Hessian at the extremum is definite, the resulting approximation is

$$\varphi(x, y) = \varepsilon \psi(\varepsilon x, \varepsilon y) \varphi_0(x, y) + \mathcal{O}_{H^s}(\varepsilon^{2/3}), \quad \omega = \omega_0 - \varepsilon^2, \quad (\text{II.2})$$

where $s > 1$ is arbitrary, φ_0 is the Bloch function at the band edge ω_0 , and $\psi = \psi(X, Y)$ in slow variables $X = \varepsilon x$ and $Y = \varepsilon y$ satisfies the stationary nonlinear Schrödinger (NLS) equation. This effective NLS equation is written in the form,

$$\alpha(\psi_{XX} + \psi_{YY}) + \beta|\psi|^2\psi = \psi, \quad (\text{II.3})$$

where $\alpha > 0$ is related to the band curvature at the point ω_0 and $\beta > 0$ is related to a norm of the Bloch function φ_0 . We note that the leading-order term $\varepsilon \psi(\varepsilon x, \varepsilon y) \varphi_0(x, y)$ has the order $\mathcal{O}_{H^s}(1)$ as $\varepsilon \rightarrow 0$ and hence expansion (II.2) shows that the perturbation term is smaller than the leading-order term in the H^s norm, where H^s is Sobolev space of square integrable functions and their derivatives up to the s -th order. When ω_0 is the (upper) edge of the semiinfinite gap, the error was shown to be $\mathcal{O}_{H^s}(\varepsilon)$ or $\mathcal{O}_{L^\infty}(\varepsilon^2)$ [9].

The main theorem of [5, 6] states that if ψ satisfies certain reversibility symmetries such as

$$\psi(X, Y) = \pm \bar{\psi}(-X, Y) = \pm \bar{\psi}(X, -Y) \quad (\text{II.4})$$

or

$$\psi(X, Y) = \pm \bar{\psi}(Y, X) = \pm \bar{\psi}(-Y, -X), \quad (\text{II.5})$$

and if the linearization of the stationary NLS equation (II.3) is non-degenerate, then a localized solution of the Gross–Pitaevskii equation (II.1) with the asymptotic expansion (II.2) exists in H^s for this ψ . In particular, the stationary NLS equation (II.3) admits the fundamental vortex of charge $m \in \mathbb{N}$,

$$\psi(X, Y) = \rho(R) e^{im\theta}, \quad R = \sqrt{X^2 + Y^2}, \quad \theta = \arg(X + iY), \quad (\text{II.6})$$

where $\rho(R) > 0$ for all $R > 0$ satisfies a certain differential equation that follows from the stationary NLS equation (II.3). Vortex solution (II.6) satisfies symmetry (II.4) and the linearization of (II.3) at this ψ is non-degenerate. Hence conditions of the main theorem in [5, 6] are validated and there exists a unique localized solutions of (II.1) continued from this ψ with the asymptotic expansion (II.2). Continuation of fundamental vortices is considered in Section III.

In the tight-binding limit of narrow spectral bands, several authors [1, 14, 15] rigorously justified that the localized states of the stationary Gross–Pitaevskii equation (II.1) can be described by the localized states of the stationary discrete nonlinear Schrödinger (DNLS) equation,

$$-(\Delta_{\text{disc}}\phi)_{m,n} - |\phi_{m,n}|^2\phi_{m,n} = \omega\phi_{m,n}, \quad (m,n) \in \mathbb{Z}^2, \quad (\text{II.7})$$

where

$$(\Delta_{\text{disc}}\phi)_{m,n} = \phi_{m+1,n} + \phi_{m,n+1} + \phi_{m-1,n} + \phi_{m,n-1} - 4\phi_{m,n}$$

and $\omega \notin \sigma(-\Delta_{\text{disc}}) = [0, 4]$. The DNLS equation can simplify numerical approximations of the continuous Gross–Pitaevskii equation but does not change properties of localized states. In particular, bifurcations of localized states are possible from the band edge $\omega = 0$ in the focusing case. Moreover, the same method of asymptotic multi-scale expansions can be adopted to the DNLS equation with the expansion

$$\phi_{m,n} = \varepsilon\psi(\varepsilon m, \varepsilon n) + o_{l^2}(1), \quad \omega = -\varepsilon^2, \quad (\text{II.8})$$

where ψ satisfies the same stationary NLS equation (II.3). A rigorous justification of the continuous NLS equation as an asymptotic model for ground states of the DNLS equation was recently developed in [3, 4]. Approximations for vortices in this context were not obtained to the best of our knowledge.

III. VORTEX FAMILY CONNECTED TO THE SPECTRAL EDGE

We compute here a family of the fundamental vortices in the DNLS equation (II.7) by using the near-edge asymptotics (II.8) with ψ given by the continuous vortex (II.6). We will also compare this behavior with the one in the Gross–Pitaevskii equation (II.1).

Choosing the vortex of charge one in the form (II.6) with $m = 1$, we compute the positive spatial profile ρ by the shooting method. We let next $\varepsilon = \sqrt{0.03}$, so that the expansion (II.8) produces an initial guess for a solution ϕ of the DNLS equation (II.7) with $\omega = -0.03$ and compute ϕ via the Newton’s method.

Next, we continue the family in the $(\omega, \|\phi\|_2^2)$ -plane using the pseudo-arclength continuation [10, 11], in which both ϕ and ω are unknowns, combined with the Newton’s method. The resulting solution family is plotted in Figure 1(a) using the computational domain $[-42, 42]^2 \subset \mathbb{Z}^2$. The starting point at $\omega = -\varepsilon^2 = -0.03$ is marked as D in Figure 1(b).

The family of vortices with charge $m = 1$ seems to fold and never reach the spectral edge contrary to the approximation (II.8). In Figure 1(b) this folding is, however, shown to be merely a numerical artifact caused by the truncation of the infinite domain \mathbb{Z}^2 . The fold location approaches the edge $\omega = \omega_0 = 0$ as the computational domain is enlarged. The family branch containing $A - D$ thus terminates at the edge if computed on domains of diverging size.

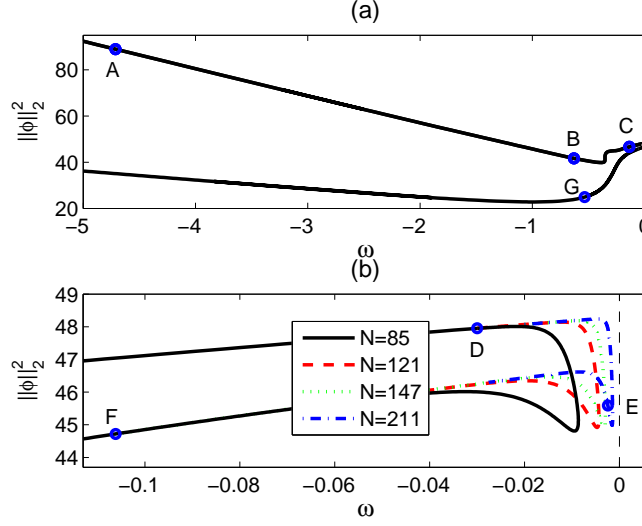


FIG. 1: Family of vortex solutions of (II.7) continued from the vortex (II.6) via the envelope approximation (II.8) at $\omega = -0.03$ (point D). (a) A fixed computational domain is used with $N = 85$. (b) Detail of the vicinity of the spectral edge for a range of sizes of the computational domain.

In the vicinity of the fold bifurcation, the solutions are inherent to the truncated domain and do not correspond to any solution of the DNLS equation (II.7) on \mathbb{Z}^2 . The fold divides the family into two branches. Only the first branch containing points A, B, C, D is a continuation of the vortex family with the asymptotics given by (II.8) with ψ as the continuous vortex (II.6). The other branch corresponds to a different family of vortex solutions.

Figure 2 shows the solutions labeled $A - G$ in Figure 1. The limiting behavior for $\omega \rightarrow -\infty$ along the branch with A and B is a vortex with a square structure with sides of length five and three active sites on each side, i.e. the excited sites are at

$$(-1, -2), (0, -2), (1, -2), (-1, 2), (0, 2), (1, 2), (-2, -1), (-2, 0), (-2, 1), (2, -1), (2, 0), (2, 1) \in \mathbb{Z}^2.$$

Along the other branch beyond the point G in the direction of decreasing ω the four solution peaks get further localized approaching single site excitations as $\omega \rightarrow -\infty$. The vortices keep charge one

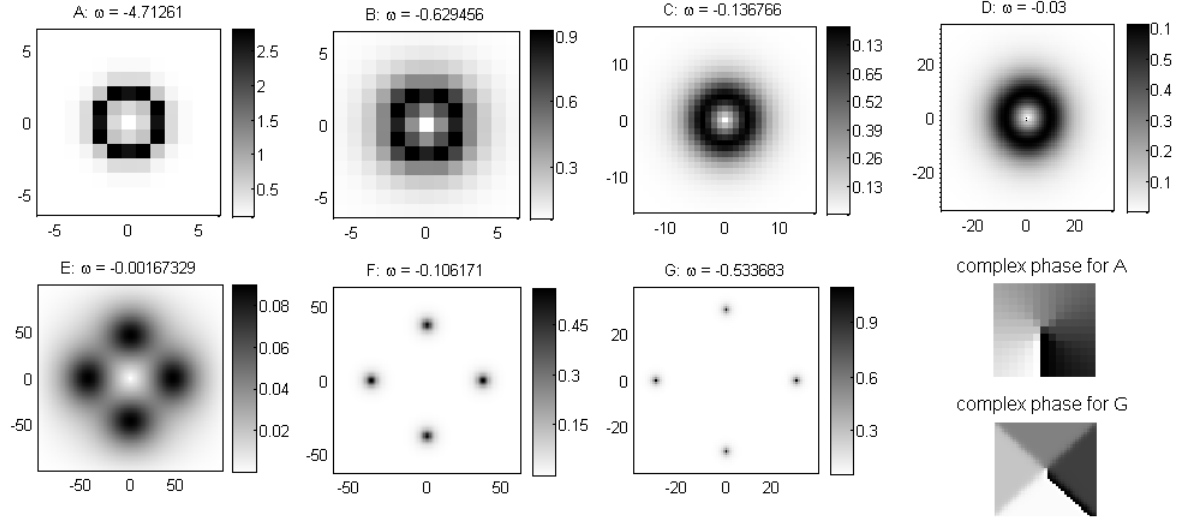


FIG. 2: A-G: Modulus of the discrete vortex solutions labeled in Fig. 1. Bottom right: plots of the complex phase for vortices A and G.

along the whole family. The complex phase for vortices A and G is plotted on the bottom right panel of Figure 2.

A similar situation arises for vortex solutions of the continuous Gross–Pitaevskii equation (II.1). In Figures 3 and 4, we present a family of vortices for

$$V(x, y) = 6 \sin^2(x) + 6 \sin^2(y),$$

which was the potential used in [22]. We consider the vicinity of the lowest spectral edge $\omega_0 \approx 4.1264$. The selected family is qualitatively similar to the discrete vortex family above and also terminates at the gap edge. The computational domain is $[-L/2, L/2]^2 \subset \mathbb{R}^2$ and the stationary equation (II.1) is discretized via central difference formulas of order 4.

The results of this section contradict the claim from [22] that no vortex families can be continued to the band edge of the Bloch spectrum. These results illustrate the validity of the main theorems from [5, 6], which point out the possibility of such continuations for solutions satisfying reversibility symmetries (II.4) or (II.5) and the non-degeneracy conditions, e.g., for the fundamental vortex solutions.

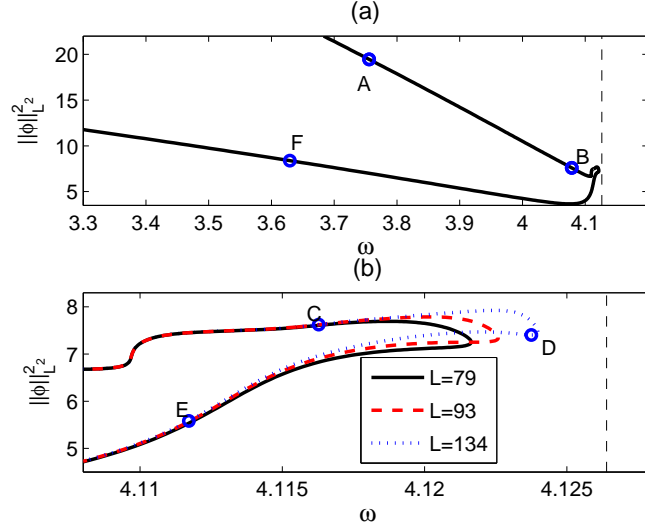


FIG. 3: Family of vortex solutions of (II.1) continued from the vortex (II.6) via the envelope approximation (II.8) at $\omega \approx 4.09$ (point B). (a) A fixed computational domain is used with $L = 93$. (b) Detail of the vicinity of the spectral edge for a range of sizes of the computational domain.

IV. QUADRUPOLE AND DIPOLE VORTEX FAMILIES DISCONNECTED FROM THE SPECTRAL EDGE

A classical example of a vortex solution of the Gross–Pitaevskii equation (II.1) and of the DNLS equation (II.7) is the quadrupole vortex with the four nearest neighbor sites excited in a square arrangement in the asymptotics $\omega \rightarrow -\infty$, i.e. with the excited sites at

$$(-1, 0), (1, 0), (0, -1), (0, 1) \in \mathbb{Z}^2.$$

For the Gross–Pitaevskii equation the excited sites are understood as locations of the single wells (minima) of the periodic potential V . We obtain this family for the DNLS equation via the initial guess

$$\phi_{m,n} = 2\delta_{m,1}\delta_{n,0} + 2i\delta_{m,0}\delta_{n,1} - 2\delta_{m,-1}\delta_{n,0} - 2i\delta_{m,0}\delta_{n,-1}, \quad (m, n) \in \mathbb{Z}^2,$$

at $\omega = -1.2$ (point D in Figure 5), where $\delta_{m,m_1}\delta_{n,n_1}$ is the Kronecker unit vector at (m_1, n_1) on \mathbb{Z}^2 . The family is then continued, once again, via the pseudo-arclength continuation combined with the Newton iteration.

In Figures 5 and 6 the family curve and several solution profiles are plotted. The computation was performed on the domains $[-N, N]^2$ with $N = 10, 16, 20, 40$ and the curves in the $(\omega, \|\phi\|_{l^2}^2)$

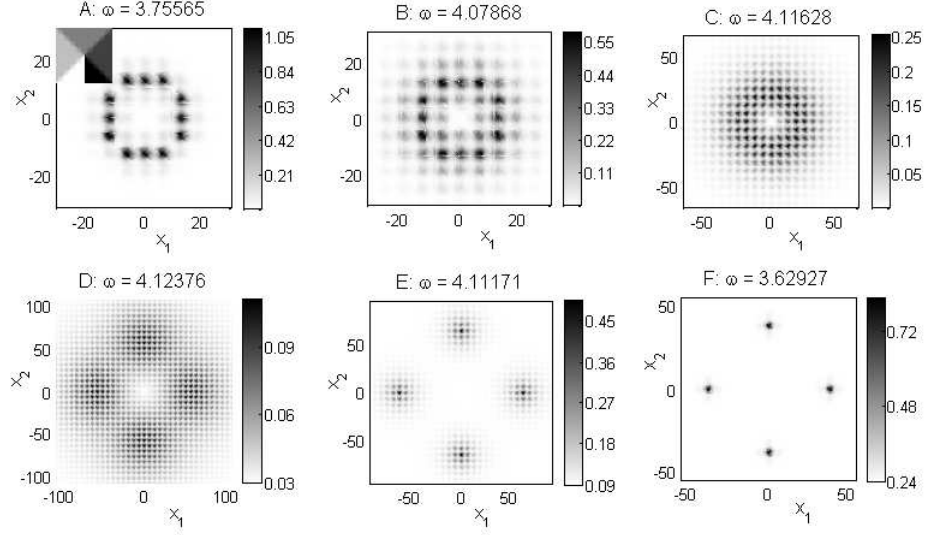


FIG. 4: Modulus of the continuous vortex solutions labeled in Fig. 3. The inset in A shows a qualitative plot of the complex phase for all vortices A-F.

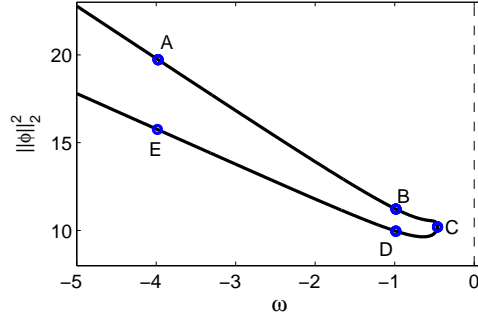


FIG. 5: Family of discrete vortex solutions continued from a quadrupole vortex and four nearest neighbor excited sites as $\omega \rightarrow -\infty$.

plane remained within the distance of $\mathcal{O}(10^{-6})$ for all these N and did not approach the edge. This family folds and does not reach the spectral edge and all its solutions remain tightly localized. It does not, therefore, contain a slowly varying solution near the band edge, which could be approximated via the envelope approximation (II.8). Qualitatively this family corresponds to the family $a - d$ in Fig. 1(a) of [22]. The branch past the fold, i.e. the branch with A and B, has as the asymptotic profile for $\omega \rightarrow -\infty$ a square vortex with excited sites at

$$(-1, -1), (-1, 0), (-1, 1), (0, 1), (1, 1), (1, 0), (1, -1), (0, -1) \in \mathbb{Z}^2.$$

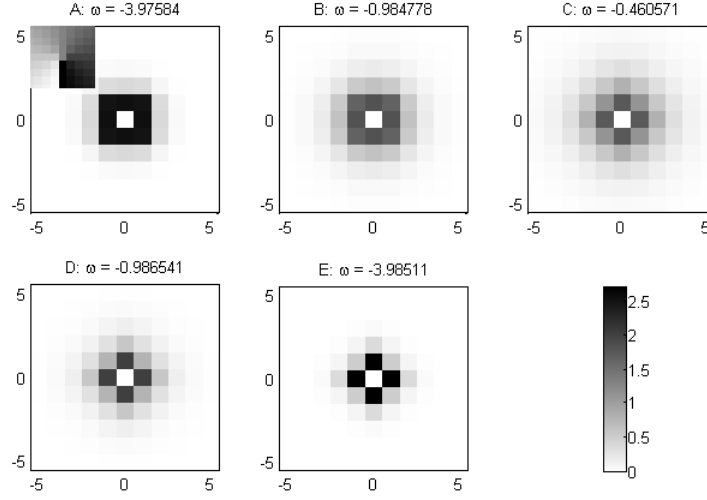


FIG. 6: Modulus of the discrete quadrupole vortex solutions labeled in Fig. 5. The inset in A shows a qualitative plot of the complex phase.

We also consider a family of real dipole solutions ϕ which are odd in the n -index and satisfy $\phi_{m,0} = 0$ for all $m \in \mathbb{Z}$. It is constructed via the “hand made” initial guess

$$\phi_{m,n} = 1.5\delta_{m,0}\delta_{n,1} - 1.5\delta_{m,0}\delta_{n,-1}, \quad (m,n) \in \mathbb{Z}^2,$$

at $\omega = -1.2$ (point D in Figure 7). The family is plotted in Figures 7 and 8. The computation was performed on the domains $[-N, N]^2 \in \mathbb{Z}^2$ with $N = 10, 15, 20, 40$ and the curves in the $(\omega, \|\phi\|_{l^2}^2)$ plane remained within the distance of $\mathcal{O}(10^{-5})$ from each other for all these N and did not approach the edge. This family contains again only tightly localized solitons and does not continue to the spectral edge either. Along the branch with points E and D the asymptotic profile for $\omega \rightarrow -\infty$ is the dipole with the excited sites $(0, -1)$ and $(0, 1)$. Along the other branch the asymptotic profile is twice as broad with the excited sites at

$$(0, -2), (0, -1), (0, 1), (0, 2) \in \mathbb{Z}^2.$$

The results of this section confirm the previous numerical results from [22], where all quadrupole vortex families have a fold bifurcation at a small distance from the band edge of the Bloch spectrum. Solutions throughout our quadrupole and dipole families remain tightly localized so that they are not compatible with the slowly varying approximation (II.8). It is, however, possible that there exist other solution families, which have a dipole or quadrupole asymptotic form as $\omega \rightarrow -\infty$ and

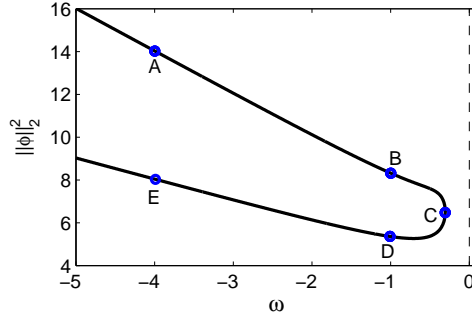


FIG. 7: Family of discrete vortex solutions continued from a dipole vortex with two nearest neighbor excited sites as $\omega \rightarrow -\infty$.

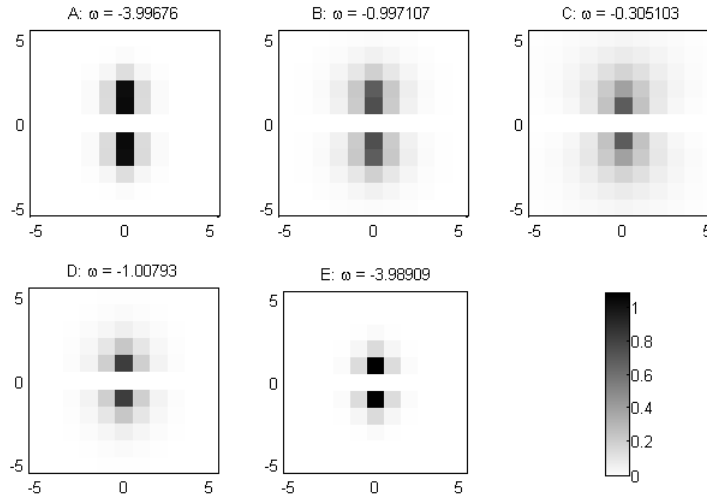


FIG. 8: Modulus of the discrete dipole vortex solutions labeled in Fig. 7.

which do bifurcate from the spectral edge. The bifurcation would be guaranteed by the results of [5, 6] if the continuous NLS equation (II.3) had dipole or quadrupole solutions, which we are not aware of.

V. CONCLUSION

We have numerically demonstrated in both the Gross-Pitaevskii equation with a two-dimensional periodic potential and the discrete nonlinear Schrödinger (DNLS) equation that there are families of fundamental vortices bifurcating from spectral edges of the Bloch wave spectrum.

This is in agreement with the analysis in [5, 6] and in contradiction with the claim in [22] that no vortex families continue to a spectral edge. Our fundamental vortex families complement the vortex families constructed in [22, 23] which all terminate at a distance from the spectral edge via a fold bifurcation.

We have also investigated families of quadrupole and dipole vortex configurations of the DNLS equation. The selected families do terminate via fold bifurcations, which are located at a small distance from the band edge, independently of the size of the computational domain. It is an open question whether there exist other families of quadrupole and dipole vortex configurations, which bifurcate from spectral edges of the Bloch wave spectrum.

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